Project H-6. Nonconventional hydrides with low H-H separations

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The project is aimed on the establishment of the relationship between structure, bonding and hydrogen storage capacities in a principally new type of metal hydrides with short H-H separations capable of reaching H-storage densities several times higher than liquid H_2.

In the recently studied new type of intermetallic hydrides, $RE_3Ni_3In_3D_4$ (Figure) [V.A. Yartys et al, *J. Alloys and Compounds*, **330-332** (2002) 132], a pair of hydrogen atoms with an unusually short H-H separation of around 1.6 Å was found. From structural point of view, in $RE_3Ni_3In_3D_4$ the appearance of short H-H distances correlates with an anisotropic uniaxial lattice expansion on hydrogenation (16 %).

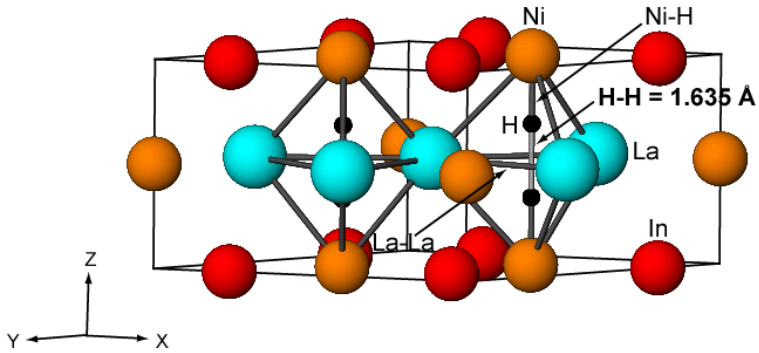

Figure. The crystal structure of $LaNiInD_{1.2}$ with a short H-H pair of 1.63 Å.

During 2003 the work was focused on studies of the RE(Ni,Cu)(In,Al) intermetallic compounds where substitutions of Ni by Cu and In by Al were expected to keep the crystal structure type (ZrNiAl) of the metal sublattice. There a pair of the RE_3TM tetrahedra having a common RE_3 face is formed, making it possible a formation of the H…H pair. The quaternary alloys prepared, $NdNi_{0,75}Cu_{0,25}In$, $NdNi_{0,5}Cu_{0,5}In$ and $NdNiIn_{0,75}Al_{0,25}$, were found to crystallise with the ZrNiAl type structure with the unit cell parameters intermediate between the ternary intermetallics NdNiIn, NdCuIn and NdNiAl. Studies of the hydrogen absorption-desorption properties and crystal structures of corresponding deuterides showed that

a) volume expansion in all cases is smaller for the substituted compounds compared to the phase transformation NdNiIn → $NdNiInD_{1.3\text{-}1.6}$;
b) the expansion is rather close to isotropic and proceeds mainly in the basal plane for the Al-containing hydride instead of along [001] for $LaNiInD_{1.3\text{-}1.6}$;
c) as a consequence, H...H pairing does not take place, in contrast to the NdNiIn-based hydride.

These data show that H...H pairing is very sensitive to the chemical behaviour of the constituents in the systems Nd(Ni,Cu)(In,Al) so when the level of substitutions exceeds 25 % both for Al and In, H...H pairing becomes impossible.

The Filter Analyzer Neutron Spectrometer at NIST is the instrument used for neutron vibrational spectroscopy. It is designed to reveal fine details of the vibrational motion of molecules acting as “fingerprints” of their surroundings in materials. Preliminary collaborative studies have been done by T.Udovic on the LaNiIn-based and related hydrides to characterise local H…H environment in these materials.

Further studies will be focused on the alloys with smaller content of substitutions allowing finally to determine critical parameters of these system which control the H...H pairing.